Consistent Analysis and Rigorous Characterization of Infinite Graphene Layers via a Subcell Frequency-Dependent FDTD Technique

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Abstract

An efficient finite-difference time-domain methodology combined with a robust subcell formulation for the precise analysis of infinite graphene sheets is introduced in this paper. The graphene surface conductivity is modeled through a volume conductivity profile, with the pertinent periodic boundary conditions applied to the unit cell’s lateral surfaces. Moreover, a set of linearly-polarized normally-incident wideband pulses excites the computational domain, while the graphene’s dispersive nature is described by an auxiliary differential equation concept. The novel algorithm is validated via several configurations and a demanding optical visibility problem, whose numerical results, compared to those of closed-form expressions, are proven very satisfactory.

1. Introduction

The aptitude to control the electronic properties of a material through an externally applied voltage has been the issue of an intensive research. Lately, this challenging goal seems to be accomplished, when graphene, a 2-D medium formed by carbon atoms arranged in a honeycomb lattice, has been isolated [1]. In graphene, a gate voltage can regulate the surface charge density, thereby controlling surface conductivity. However, the most intriguing merit is that electrons in its interior behave as massless relativistic particles (i.e. Dirac fermions) and exhibit ballistic transport. This is attributed to the fact that the energy-momentum relationship becomes linear, instead of quadratic, for the low energies near the six corners of the 2-D hexagonal Brillouin zone. Actually, graphene, in its most qualitative form, has been produced by the mechanical exfoliation of graphite. Since then, many processes have been proposed for high quality graphene [2, 3]. Among its numerous applications, one can discern the use in the advancement of transistors or integrated circuits with graphene nanoribbons as well as in the fabrication of transparent electrodes required for touch screens, liquid crystal displays and organic photovoltaic cells along with various setups for modern devices in the microwave regime [4-8].

It is the purpose of this paper, to present a 3-D frequency-dependent finite-difference time-domain (FDTD) methodology based on an enhanced subcell concept for the accurate characterization of infinite graphene layers, possibly arranged in arbitrary geometric patterns. Extracting the necessary conductivity model of graphene through quantum mechanical analysis, the new technique establishes a consistent discretization which takes into account its inherent properties and structural peculiarities, thus enabling reliable interpretations. Also, graphene is handled as a complex isotropic volume conductivity, whose dispersive nature is efficiently incorporated via an auxiliary differential equation (ADE) algorithm to allow an explicit implementation. In this context, the material under study occupies a fraction of an elementary cell in the computational domain, while infinite sheets are realized by a set of periodic boundary conditions (PBCs) applied to lateral surfaces. Finally, the discretized space is excited with normally-incident broadband electromagnetic pulses of linear polarization, launched by a properly modified total-field/scattered-field (TF-SF) formulation. The proposed method is verified in terms of different graphene setups, including a problem of optical visibility, and simulations are compared to the solutions of closed-form relations with a promising agreement, which permits its potential use as a reliable design/optimization tool for many realistic applications, where analytical formulas cannot be extracted.

2. Accurate Graphene Surface Conductivity Models

Let us consider the configuration of Fig. 1a, where the graphene layer is modeled by an infinitesimally thin conductivity surface, located between two arbitrary dielectrics with constitutive parameters \( (\varepsilon_1, \mu_1) \) and \( (\varepsilon_2, \mu_2) \), respectively. The graphene’s surface anisotropic conductivity, in its general form, is given by the dyadic [5]

\[
\tilde{\sigma}(\omega, \mu_0, E_0, \Gamma, T, B_0) = \tilde{\sigma}_x \sigma_x + \tilde{\sigma}_y \sigma_y + \tilde{\sigma}_z \sigma_z + \gamma \tilde{\sigma}_n,
\]

and depends on the radian frequency \( \omega \), the chemical potential \( \mu \), (controlled by an electrostatic bias field \( E_0 \)), a phenomenological scattering rate \( \Gamma \), the temperature \( T \), and an applied magnetostatic bias field \( B_0 \). Herein and for the sake of
simplicity, we assume that \( B_\Omega = 0 \), a fact which renders the conductivity isotropic (i.e. \( \sigma_g = \sigma_\alpha = 0 \)) and, now, described by
\[
\sigma_{\alpha\alpha} = \sigma_{\alpha\gamma} = \sigma_{\gamma\gamma} = \sigma_{\gamma\alpha} = \frac{\mu c}{\pi \hbar^2 (\omega - j 2\Gamma)} \int_0^\infty \left[ \frac{\partial f_\alpha(e)}{\partial e} - \frac{\partial f_\gamma(e)}{\partial e} \right] de - \frac{\mu c}{\pi \hbar^2 (\omega - j 2\Gamma)} \int_0^\infty \frac{f_\alpha(e) - f_\gamma(e)}{\pi \hbar^2 (\omega - j 2\Gamma)^2 - 4(e/\hbar)^2} de, \tag{2}
\]
where \( e \) is the electron charge, \( \hbar = h/2\pi \) is the reduced Planck’s constant, \( f(e) = \{\exp[(e - \mu_c)/k_BT] + 1\}^{-1} \) is the Fermi-Dirac distribution, and \( k_B \) the Boltzmann’s constant. Note that the first integral in (2) accounts for the intraband contributions, while the second integral for the interband ones. After some algebra, these terms can be written as
\[
\sigma_{\alpha\alpha}(\omega, \mu_c, \Gamma, T) = -\frac{j\hbar^2 k_BT}{\pi \hbar^2 (\omega - j 2\Gamma)} \left[ \frac{\mu_c}{k_BT} + 2\ln(e^{\mu_c/T} + 1) \right] \quad \text{and} \quad \sigma_{\alpha\gamma}(\omega, \mu_c, \Gamma, T) = -\frac{j\hbar^2}{4\pi \hbar} \ln \left[ \frac{2\mu_c}{\mu_c - (\omega - j 2\Gamma)\hbar} \right], \tag{3}
\]
where for the latter the \( k_BT << |\mu_c|, \hbar \omega \) constraint has been considered. Also, \( \mu_c \) can be acquired via the carrier density \( n_e \)
\[
n_e = \frac{2}{\pi \hbar^2 v_F^2} \int_0^\infty e^{\left[ f_\alpha(e) - f_\gamma(e) + 2\mu_c \right]} de, \tag{4}
\]
for \( v_F = 9.5 \times 10^5 \text{ m/s} \) the Fermi velocity. In this manner, the prior relations provide a complex conductivity \( \sigma = \sigma' + j\sigma'' \). It is stressed that, due to its negligible contribution at the frequency spectrum examined in this work, the interband term is ignored, so leading to the more convenient expression of \( \sigma = \sigma_g = \sigma_{\alpha\alpha} \).

3. Formulation of the Explicit Subcell Frequency-Dependent Algorithm

For the development of the 3-D FDTD methodology, the graphene sheet is supposed to be located on the z-plane. The domain is discretized in a lattice of periodic unit cells with simple Floquet PBCs applied to x and y lateral surfaces, whereas the structure is excited by wideband pulses of normal incidence via a suitably adjusted version of the TF-SF formulation [9]. Due to the periodicity of the problem, coupled with the excitation type, the fields on the outer boundaries must be equal. On the other hand, the domain along the z direction is truncated by an 8-cell perfectly matched layer (PML), as shown in Fig. 1b. To precisely model the thin graphene layer, a modified subcell scheme is introduced, according to which the medium under study occupies only a portion (with a volume percentage \( \alpha \)) of the Yee cell. Since the conventional FDTD algorithm can not sufficiently treat surface conductivities, \( \sigma_{\alpha\alpha} \) in (3) is transformed to its volume counterpart \( \sigma_{\alpha\alpha} \) via the \( \sigma_{\alpha\alpha} = \sigma(\alpha\Delta z) \) relation. Based on the subcell concept [10], electric component \( E_z \) in all cells containing graphene is split into two parts, \( E_z^{\text{gr}} \) (graphene area) and \( E_z^{\text{PML}} \) (rest of the cell), as it is not continuous across the material interface. This approach is, herein, further enhanced by splitting magnetic component \( H_z \) into \( H_z^{\text{PML}} \) and \( H_z^{\text{surf}} \) as well. Conversely, tangential quantities do not require an analogous treatment, since they are continuous across the interface. Finally, to model the dispersive nature of \( \sigma_{\alpha\alpha} \), an ADE method is employed. Hence, if \( \sigma_{\alpha\alpha} \) is expressed as
\[
\sigma_{\alpha\alpha} = -\frac{e^2 k_BT}{2 B_\Omega jZ}, \quad \text{where} \quad A = e^2 k_BT \left[ \frac{\mu_c}{k_BT} + 2\ln(e^{\mu_c/T} + 1) \right], \quad B = \pi h^2, \quad Z = 2\pi h^2 \Gamma, \tag{5}
\]
the conductivity current \( \mathbf{J} \) inside the graphene layer satisfies the vector relation
\[
\mathbf{J} = \sigma_{\alpha\alpha} \mathbf{E} \Rightarrow Bj\omega \mathbf{J} + Z\mathbf{J} = A\mathbf{E} \Rightarrow B\partial \mathbf{J} + Z\mathbf{J} = A\mathbf{E}, \tag{6}
\]
where the dot denotes the frequency domain. Observe that the graphene subcell is assumed to be entirely inside material 1 as depicted in Fig. 1a, thus sharing its constitutive parameters, namely \( \varepsilon_i \) and \( \mu_i \). Similar equations can be derived in the case where the subcell is located inside material 2. Application of Ampère’s law in an arbitrary Yee cell containing
the graphene subcell yields the update of the electric field. Concentrating on \(E_x\), its time-advancement becomes
\[
\frac{\varepsilon_1 + \varepsilon_2}{2} \frac{\partial E_x}{\partial t} + \alpha J_x = \alpha \frac{\partial H_z}{\partial y} + (1 - \alpha) \frac{\partial H_x}{\partial z} \Rightarrow E_x^{(1/2)} = E_x^{(0)} + \frac{\alpha 2 \Delta \varepsilon_1}{\varepsilon_1 + \varepsilon_2} J_x^{(1/2)} + \frac{2 \Delta \varepsilon_1}{\varepsilon_1 + \varepsilon_2} \left[ H_z^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} - H_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} + \right. \\
\left. (1 - \alpha) H_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} - H_z^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} \right], \tag{7}
\]
for \(k^z\) the \(z\) coordinate of the graphene subcell. The conductivity current term \(J_x\) is evaluated via (6) in terms of
\[
J_x^{(1/2)} = \frac{2 B - Z \Delta t}{2 B + Z \Delta t} J_x^{(0)} + \frac{2 \Delta \varepsilon_1}{2 B + Z \Delta t} E_x^{(1/2)}, \tag{8}
\]
with equivalent equations holding for \(E_y\). In the prior, \(E_x\) is evaluated through a standard FDTD expression, while \(E_y\) is calculated by (7) and (8) on condition that \((\varepsilon_1 + \varepsilon_2)/2\) is replaced by \(\varepsilon_1\) and \(\alpha = 1\). On the other hand, for the magnetic field component, we apply Faraday’s law. Therefore, the update of \(H_x\) component, for instance, is conducted by
\[
\mu_1 + \mu_2 \frac{\partial H_x}{\partial t} = -\alpha \frac{\partial E_x}{\partial y} - (1 - \alpha) \frac{\partial E_x}{\partial z} \Rightarrow H_x^{(1/2)} = H_x^{(0)} + \frac{\alpha 2 \Delta \mu_1}{\mu_1 + \mu_2} + \frac{2 \Delta \mu_1}{\mu_1 + \mu_2} \left[ E_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} - E_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} + \right. \\
\left. (1 - \alpha) E_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} - E_x^{(1/2)} \int_{j=1, \lambda = \frac{1}{2}}^{j=\lambda + 1, \lambda = \frac{1}{2}} \right], \tag{9}
\]
with a similar set of equations for \(H_y\). Again, \(H_y\) is obtained via the usual FDTD expressions and \(H_{ij}\) is computed by (9) with \(\mu_1\) substituting the \((\mu_1 + \mu_2)/2\) term and \(\alpha = 1\).

4. Numerical Results

To certify the assets of our algorithm, the 3-D computational space is excited with normally-incident and linearly-polarized TEM waves along the \(x\)-axis. The excitation follows a Gaussian temporal variation according to \(E_x(t) = E_0 \exp[(t - T_o)/(2T_0)^2]\), with \(T_o\) and \(T_0\) pertinently selected to define a bandwidth of 2 THz, which provides a really challenging spectrum for the technique’s overall efficiency. Moreover, spatial increments are set to \(\Delta x = \Delta y = \Delta z = \lambda_{\text{min}}/20\), for \(\lambda_{\text{min}}\) the wavelength corresponding to the maximum excited frequency, while the portion of the cell occupied by graphene is \(\alpha = 0.1\). For the sake of reliability, all results – regarding the reflection and transmission coefficient – are, respectively, compared to closed-form expressions \(R = (\eta_2 - \eta_1 - \eta_1 \eta_2)/(\eta_2 + \eta_1 + \eta_1 \eta_2)\) and \(T = 2 \eta_2/(\eta_2 + \eta_1 + \eta_1 \eta_2)\), where \(\eta_\alpha = (\mu_\alpha/\varepsilon_\alpha)^{1/2}\). Hence for the first application, a graphene layer \((\mu_\alpha = 0.2\ \text{eV}, T = 300K, \Gamma = 0.065\ \text{meV})\), is placed atop the interface of two dielectrics with \(\varepsilon_1 = \varepsilon_0\) and \(\varepsilon_2 = 3\varepsilon_0\) or \(\varepsilon_0\). Figure 2 presents the outcomes, which clearly indicate the high accuracy (see inlet zoom) of the proposed technique, despite the very broad frequency range. Equally satisfactory are the results of Fig. 3 for the second problem, where \(\Gamma\) is increased to 6.6 meV and \(\varepsilon_2 = 4\varepsilon_0\) or \(10\varepsilon_0\).

![Fig. 2. (a) Magnitude and (b) phase of the transmission coefficient for two graphene configurations and \(\varepsilon_1 = \varepsilon_0, \varepsilon_2 = 3\varepsilon_0\) or \(\varepsilon_0\).](attachment:image.png)

The applicability of our method is further verified via the setup of Fig. 1c; a graphene monolayer surface located atop a 1\(\mu\)-m thick SiC wafer, excited by \(E_x(t) = \cos(2\pi f_0 t)\exp[(t - T_o)/(2T_0)^2]\) at optical frequencies, where the imaginary part of graphene surface conductivity becomes insignificant and the real part is \(\sigma = 6.085 \times 10^5\ \text{S}\) (acquired from the \(\sigma_{\text{inter}}\) term). From the ideas of [4], the reflection coefficient of the structure – for \(\alpha = a_1 = a_2 = 0, s = 1\ \text{mm}, k\) the wavenumber, \(\varepsilon_{\text{SiC}}\) the SiC relative dielectric constant, and \(g = 2.55\%\) the absorption coefficient of graphene – can be obtained through

\[
\frac{\varepsilon_{\text{SiC}}}{\varepsilon_{\text{SiC}} + 1} ...
Fig. 3. (a) Magnitude and (b) phase of the transmission coefficient for two graphene configurations and $\varepsilon_1 = \varepsilon_0$, $\varepsilon_2 = 4\varepsilon_0$ or $10\varepsilon_0$.

Fig. 4. (a) Reflection coefficient and (b) snapshot stages of electric field magnitude for the SiC wafer graphene arrangement.

$$R = \frac{C \sqrt{\varepsilon_r} \cos a - D(1 - g \cos a) \cos a}{C \sqrt{\varepsilon_r} \cos a + D(1 + g \cos a) \cos a}, \quad \text{with } C = \cos a \cos X_s - j \sqrt{\varepsilon_r} \cos a_j \sin X_s, \quad D = -j \cos a_j \sin X_s + \sqrt{\varepsilon_r} \cos a_j \cos X_s. $$

Figure 4a illustrates the comparison between numerical and closed-form outcomes, where the achieved accuracy is, again, notable, although spatial resolution has been kept relatively small. Finally, Fig. 4b confirms the modeling competences of the method through the smoothness of electric field snapshots at different stages of the simulation. From the results of this section, it becomes apparent that the proposed technique can be considered as a trustworthy means for the analysis, design, and optimization of diverse real-world graphene realizations, for which analytical solutions do not exist.

5. Conclusion

A fully 3-D set of dispersive FDTD algorithms for the accurate investigation of wave interactions with infinite graphene sheets has been presented in this paper. The novel method incorporates an effective subcell process and accordingly tuned PBCs. Results and comparisons for various cases substantiate the technique’s merits for a wide frequency range.

6. References